

2005

Semantic Web & Semantic Web Services: Applications in Healthcare And Scientific Research

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LSDIS

Large Scale Distributed Information Systems



University of Georgia
Computer Science Department

Semantic Web & Semantic Web Services: Applications in Healthcare and Scientific Research

International IFIP Conference on Applications of Semantic Web

(IASW2005), Jyväskylä, Finland, August 26, 2005

Keynote: Part II

Amit Sheth

LSDIS Lab, Department of Computer Science,
University of Georgia

<http://lsdis.cs.uga.edu>



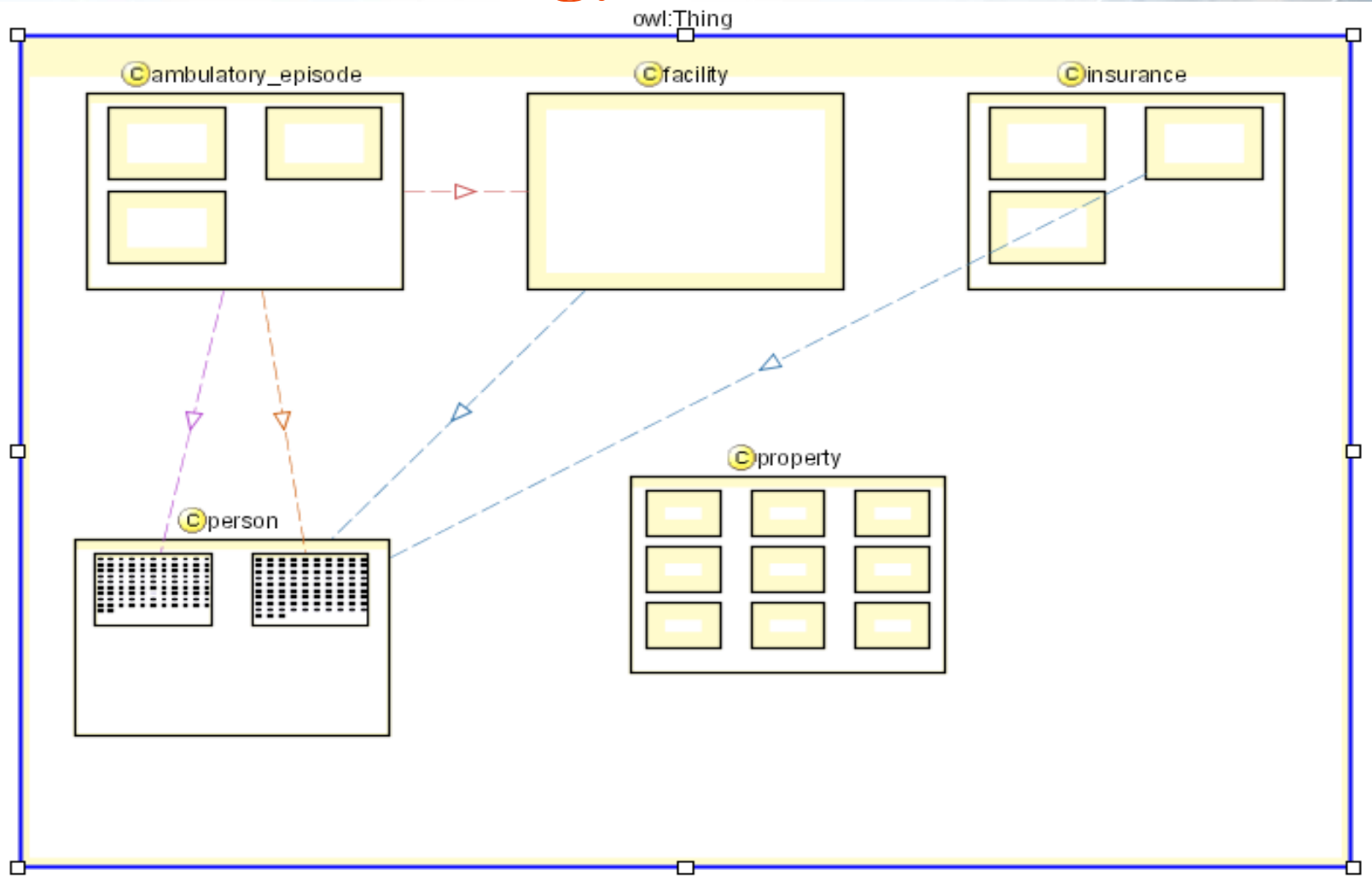
Active Semantic Document

A document (typically in XML) with

- Lexical and Semantic annotations (tied to ontologies)
- Actionable information (rules over semantic annotations)

Application: Active Semantic Patient Record for Cardiology Practice

Practice Ontology





Practice Ontology

practice_ontology Protégé 3.0 (file:IC:\javaDrugOntWs\resource\practice_ontology.pprj, OWL Files (.owl or .rdf))

File Edit Project OWL Wizards Code Window Help Jambalaya

protégé

OWLClasses Properties Forms Individuals Metadata Jambalaya

SUBCLASS RELATIONSHIP

For Project: practice_ontology

Asserted Hierarchy

- owl:Thing
 - ambulatory_episode
 - ancillary
 - encounter
 - event
 - facility
 - insurance
 - insurance_carrier
 - insurance_plan
 - insurance_policy
 - person
 - patient
 - practitioners
 - property
 - ambulatory_episode_property
 - facility_property
 - insurance_carrier_properties
 - insurance_plan_property
 - insurance_policy_properties
 - patient_property
 - practitioner_property
 - provider_group_property
 - specialty_property

CLASS EDITOR

For Class: patient (instance of owl:Class)

Name: SameAs DifferentFrom

patient

rdfs:comment

Annotations

Property	Value	Lang
----------	-------	------

Asserted **Inferred**

Asserted Conditions

NECESSARY & SUFFICIENT

NECESSARY

person

Properties

- has_phone_number (single String)
- has_race (single String)
- has_religion (single String)
- has_served_for_military (single String)
- has_ssn (single String)
- has_state (single String)
- has_time (single time)
- has_year (single String)
- has_zip_code (single String)

Disjoints

Logic View Properties View

start

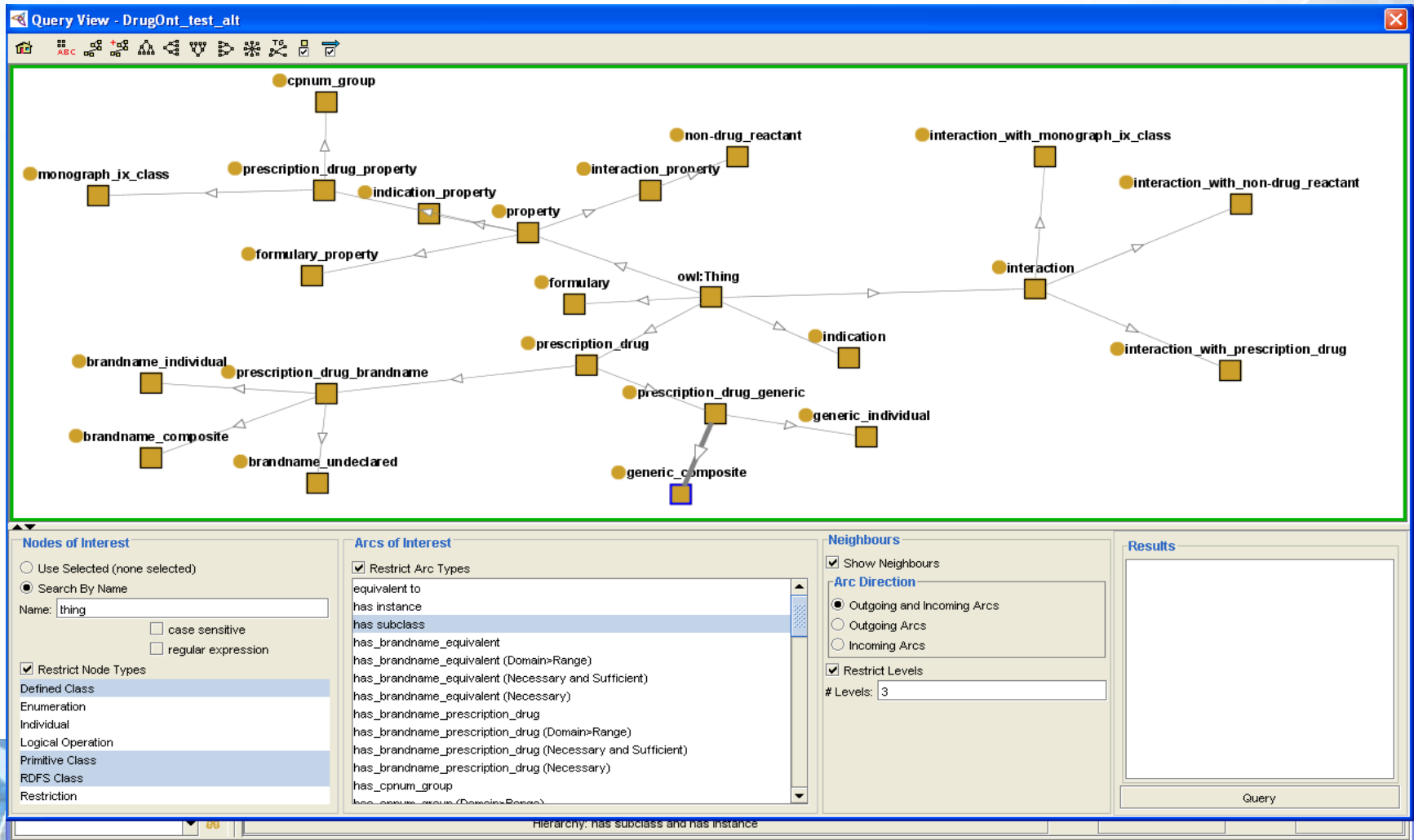
Google - Mozilla Firefox Gmail - AHC slides - M... Mozilla Firefox Protege.exe

practice_ontology Pr... Microsoft PowerPoint ... Jasc Paint Shop Pro - ...

10:36 AM Sunday 8/21/2005

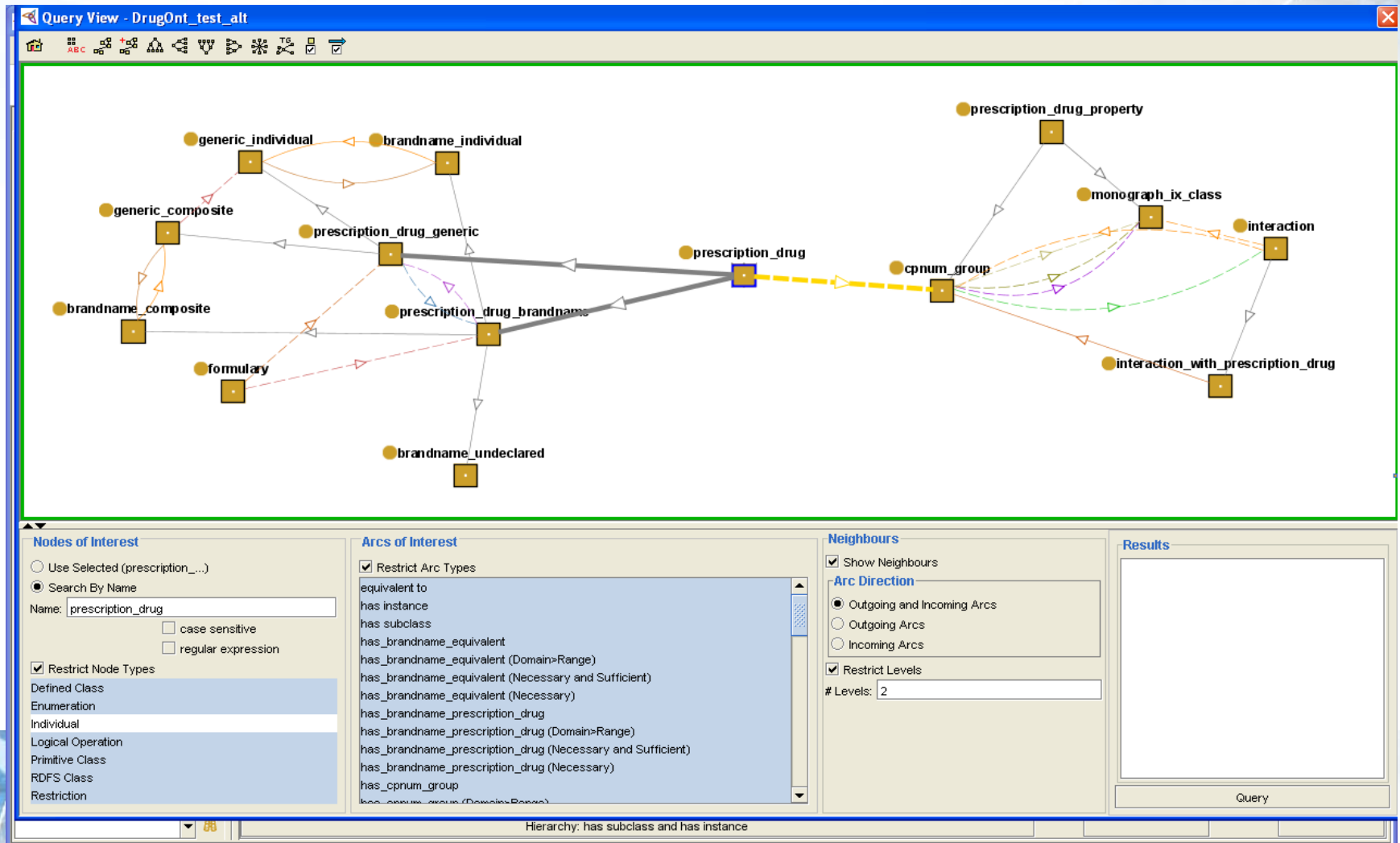


Drug Ontology Hierarchy (showing is-a relationships)





Drug Ontology showing neighborhood of *PrescriptionDrug* concept



Two of the most active
very (which builds upon






Active Semantic Doc with 3 Ontologies

AHC Acct No: 222222 - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Back Forward Stop Home Search Favorites

Address C:\lex\final.xml Go Links



Athens Heart Center
Shyam "Sham" Prabhakar
 333Dogs Drive, Apt 604, ATHENS, GA 30606
 SSN: 222-22-2222 MR #: 222222 Sex: M DOB: 05/07/1970 Age: 33

30606 Phone: 706-208-9700 Fax: 706-208-0806 Visit on 07/29/2005

Referred doctor from Practice Ontology

Office Visit Note - Complete History & Physical

Other Physicians: David Almand, M.D. E Timothy Gibson, M.D. E Alfredo Alarcon, E
 Emergency Medicine (770) 922-3023 Family Practice 706-227-2027 (404) 256-5212

Problem List:

3. Backache unspecified E
4. Hypercholesterolemia E
5. Chest Pain E
 - A. Hypertension E
 - B. Shortness of Breath.
6. Dilated cardiomyopathy gthghjg
7. Abnormal ECG
9. Acute Glomerulonephritis with other specified Pathological Lesion in Kidney E
10. Something
11. Chest Pain E

ICD9 codes from Diagnosis Procedure Ontology

Lexical annotation

Chief Complaint: Follow up of abdominal aortic aneurysm, angina, aortic stenosis, aortic valve replacement, dental clearance, and atrial fibrillation status post abnormal stress test. Cardiac clearance for aneurysm removal. Follow up of recent hospitalization at BJC - Commerce for atrial fibrillation.

History of Present Illness: Mr. Prabhakar is a 35 year old patient of Dr David Almand, Dr Timothy Gibson, and Dr Alfredo Alarcon. He was admitted to Ty Cobb Memorial by Dr. Alfredo Alarcon for bradycardia. He was found to have complete heart block. He was treated with mitral valve replacement. And he did not respond well. The patient was then transferred to Emory. He was admitted to Emory by Dr. Timothy Gibson for angina. He was found to have atrial fibrillation and complete heart block. He was treated with cholecystectomy and he responded well. The patient was then transferred to St. Mary's Hospital. He is here today for follow up management of arrhythmia, atrial fibrillation, and ICD function. Since his last visit new problems have developed. He is taking his medications as prescribed. There appear to be possibly some side effects related to the medications. Overall, he believes that his arrhythmia, atrial fibrillation, and ICD function is poorly controlled. He is here today for follow up management of cardiomegaly and coronary artery disease. Since his last visit no new problems have developed. He is taking his medications as prescribed. There appear to be possibly some side effects related to the medications. Overall, he believes that his cardiomegaly and coronary artery disease is stable. The chest pain is associated with itchy. He reports that his chest pain is aggravated by bending. The chest pain is relieved by belching. The patient reports this morning with her spell. Dizziness is associated with palpitations. He states that this symptom is aggravated by activity, bending, and high blood pressure. The dizziness is relieved by sitting down. He states that the palpitations are aggravated by position changes.

Current Medications	Medications After Visit

Done My Computer



Active Semantic Doc with 3 Ontologies

AHC Acct No: 222222 - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Back Forward Stop Home Search Favorites

Address C:\lex\final.xml

Current Medications	Medication
Intropin injection 40mg/ml, 1 inj qd I E	Intropin injection 40mg/ml, 1 inj qd I E
Tasmar tablets 200mg, 1 tab qd I E	Advil 100mg/5ml, 1 susp qd F E
	Tasmar tablets 200mg, 1 tab qd I E
	Tylenol extended release 300mg, 1 tab er qd A F E

Pharmacy: Carson's Commerce Drug Company Phone: 706-754-4128 Phone: 706-335-3111

Allergies: AMPICILLIN, IVP DYE, PENICILLIN, TYLENOL

Past Medical History: No past trauma

Family History: Mr. Prabhakar has a positive family history of coronary artery disease. The patient's **crap2** is deceased.

Psychosocial: Mr. Prabhakar resides in a apartment home. He is lives with her daughter to hkkd. He has excellent social support.

Life History:

Review of Systems:

General Patient reports daily chills associated with chest pain. These symptoms have not been worked up by his primary care physician. Patient reports recent unintentional weight gain. This problem has not been worked up by his primary care physician.!!error!! Patient reports recent onset of severe trouble falling asleep. This problem has been working up by his primary care physician.

HEENT The patient reports migraine headache.

Genitourinary Patient denies dysuria. Patient complains of recent onset of hematuria. Patient complains of chronic presence of hesitancy. Patient denies dribbling. Patient complains of recent onset of burning with urination.

Hematologic Patient reports history of blood transfusion as a result of anemia. Patient reports he did experience a transfusion reaction.

Skin Patient reports frequent of mild pruritis associated with weakness. This problem has been worked up by the patient's dermatologist. Patient reports a walnut-sized keratosis that is located over the entire body.

Psychiatric Patient admits to a history of panic attacks that is currently managed by common mental health. His symptoms are felt to be not under control.

Vital Signs: Height: 170 Weight: 280 lbs BP: 120/80 Pulse: 80 Respirations: 20

Physical Examination:

General The patient appears the stated age.

Formulation Recommendation Using Insurance ontology

Drug Interaction using Drug Ontology

Drug Allergy

Done My Computer



Explore neighborhood for drug *Tasmar*

Explore: Drug *Tasmar*

AHC Acct No: 222222 - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Back Forward Stop Search Favorites

Address C:\lex\final.xml

Current Medications	
Intropin injection 40mg/ml, 1 inj qd I E	Intropin injection 40mg/ml, 1 inj qd I E
Tasmar tablets 200mg, 1 tab qd I E	Advil 100mg/5ml, 1 susp qd F E
	Tasmar tablets 200mg, 1 tab qd I E
	Tylenol extended release 650mg, 1 tab er qd A F E

Pharmacy: Carson's
Commerce Drug Company
Phone: 706-754-4128
Phone: 706-335-3111

Allergies: AMPICILLIN, IVP DYE, PENICILLIN, TYLENOL

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Vital Signs: Height: 170 Weight: 280 lbs BP: 120/80 Pulse: 80 Respirations: 20

Physical Examination:

General The patient appears the stated age.

Done My Computer



Explore neighborhood for drug *Tasmar*

Query View - DrugOnt_test_alt

Semantic browsing and querying-- perform decision support (how many patients are using this class of drug, ...)

Nodes of Interest

☐ Use Selected (none selected)

☒ Search By Name

Name:

☐ case sensitive

☐ regular expression

☒ Restrict Node Types

Defined Class

Enumeration

Individual

Logical Operation

Primitive Class

RDFS Class

Restriction

Arcs of Interest

☒ Restrict Arc Types

equivalent to

has instance

has subclass

has_brandname_equivalent

has_brandname_equivalent (Domain>Range)

has_brandname_equivalent (Necessary and Sufficient)

has_brandname_equivalent (Necessary)

has_brandname_prescription_drug

has_brandname_prescription_drug (Domain>Range)

has_brandname_prescription_drug (Necessary and Sufficient)

has_brandname_prescription_drug (Necessary)

has_cpnum_group

has_cpnum_group (Domain>Range)

Neighbours

☒ Show Neighbours

Arc Direction

☒ Outgoing and Incoming Arcs

☐ Outgoing Arcs

☐ Incoming Arcs

☒ Restrict Levels

Levels:

Results

Query



Bioinformatics Apps & Ontologies

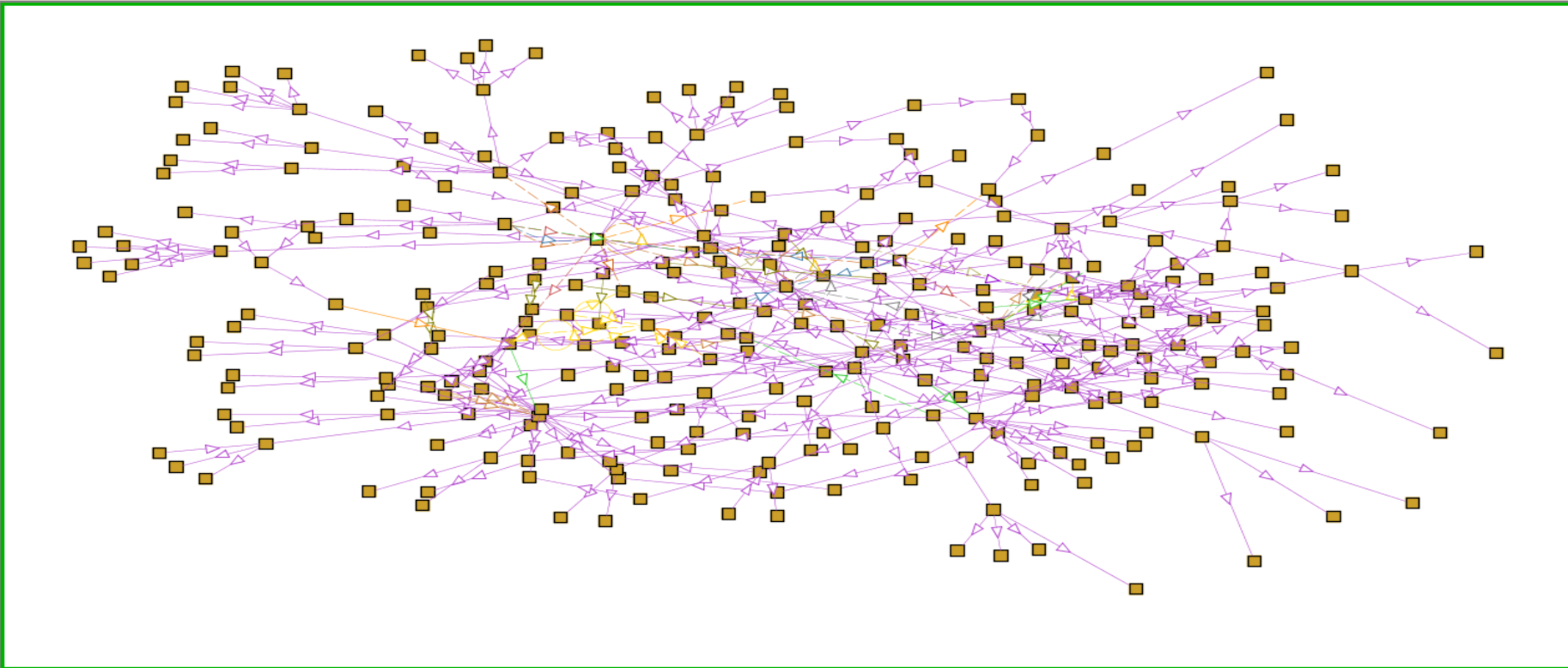
- **GlycO**: A domain ontology for glycan structures, glycan functions and enzymes (embodying knowledge of the structure and metabolisms of glycans)
 - Contains 770 classes and 100+ properties – describe structural features of glycans; unique population strategy
 - URL: <http://lsdis.cs.uga.edu/projects/glycomics/glyco>
- **ProPreO**: a comprehensive process Ontology modeling experimental proteomics
 - Contains 330 classes, 40,000+ instances
 - Models three phases of experimental proteomics* – Separation techniques, Mass Spectrometry and, Data analysis; URL: <http://lsdis.cs.uga.edu/projects/glycomics/propreo>
- Automatic semantic annotation of high throughput experimental data (**in progress**)
- Semantic Web Process with WSDL-S for semantic annotations of Web Services
 - <http://lsdis.cs.uga.edu> -> Glycomics project (funded by NCRR)

GlycO – A domain ontology for glycans

Large Scale Distributed Information Systems



Query View - GlycO_7-26-05_pop_test_4



Nodes of Interest

☐ Use Selected (none selected)
☒ Search By Name

Name:

☐ case sensitive
☐ regular expression

☒ Restrict Node Types

- Defined Class
- Enumeration
- Individual
- Logical Operation
- Primitive Class
- RDFS Class
- Restriction

Arcs of Interest

☒ Restrict Arc Types

- adds_glycosyl_residue
- adds_glycosyl_residue (Domain>Range)
- adds_glycosyl_residue (Necessary and Sufficient)
- adds_glycosyl_residue (Necessary)
- binds-epitope
- binds-epitope (Domain>Range)
- binds-epitope (Necessary and Sufficient)
- binds-epitope (Necessary)
- binds_haplin
- binds_haplin (Domain>Range)
- binds_haplin (Necessary and Sufficient)
- binds_haplin (Necessary)
- contains_functional_group

Neighbours

☒ Show Neighbours

Arc Direction

☒ Outgoing and Incoming Arcs
☐ Outgoing Arcs
☐ Incoming Arcs

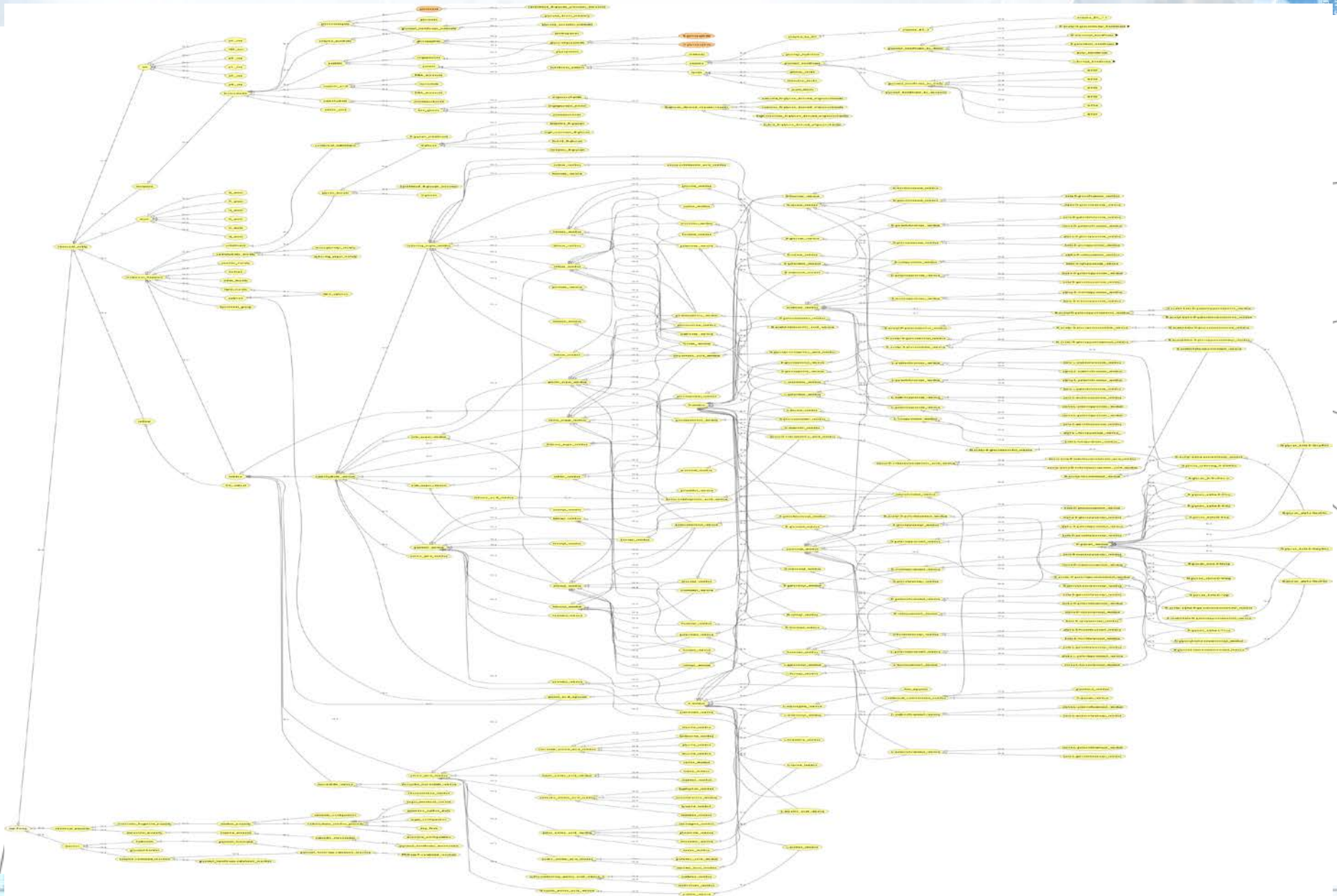
☒ Restrict Levels

Levels:

Results

Query

Slide 4 of 4 Default Design English (U.S.)



Structural modeling issues in GlycO



- Extremely large number of glycans occurring in nature
- But, frequently there are small differences structural properties
- Modeling all possible glycans would involve significant amount of redundant classes
- Redundancy results in often fatal complexities in maintenance and upgrade

Two of the most active
very (which builds upon
TEOR's Samana Web



N. Takahashi and K. Kato, *Trends in Glycosciences and Glycotechnology*, 15: 235-251

glycan-0816a04 Protégé 2.1 beta (file: C:\Program%20Files\Protege_2.1_beta\projects\glycomics\glycan-0816a04.pprj, OWL Files)

Project Edit Window OWL Help

OWLClasses Properties Forms Individuals Metadata Jambalaya

Subclass Relationship

Asserted Hierarchy

- N-glycan_residue
 - N-glycan_alpha-Fuc_20
 - N-glycan_alpha-Fuc_25
 - N-glycan_alpha-Fuc_27
 - N-glycan_alpha-Fuc_50
 - N-glycan_alpha-Gal_38
 - N-glycan_alpha-Gal_42
 - N-glycan_alpha-Gal_44
 - N-glycan_alpha-Gal_48
 - N-glycan_alpha-Gal_57
 - N-glycan_alpha-Gal_58
 - N-glycan_alpha-Gal_59
 - N-glycan_alpha-Gal_60
 - N-glycan_alpha-Gal_61
 - N-glycan_alpha-Glc_51
 - N-glycan_alpha-Man_11
 - N-glycan_alpha-Man_15
 - N-glycan_alpha-Man_16
 - N-glycan_alpha-Man_19
 - N-glycan_alpha-Man_30
 - N-glycan_alpha-Man_4**
 - N-glycan_alpha-Man_7
 - N-glycan_alpha-Man_8
 - N-glycan_alpha-NeuAc_23
 - N-glycan_alpha-NeuAc_31
 - N-glycan_alpha-NeuAc_32
 - N-glycan_alpha-NeuAc_35
 - N-glycan_alpha-NeuAc_36
 - N-glycan_alpha-NeuAc_40
 - N-glycan_alpha-NeuAc_41
 - N-glycan_alpha-NeuAc_43
 - N-glycan_alpha-NeuAc_46
 - N-glycan_alpha-NeuAc_47

N-glycan_alpha-Man_4 (type=owl:Class)

Name: N-glycan_alpha-Man_4

rdfs:comment

Annotations

Property	Value	Lang
----------	-------	------

Asserted Inferred

Asserted Conditions

NECESSARY & SUFFICIENT

NECESSARY

- alpha-D-mannopyranosyl_residue
- N-glycan_residue
- \exists has_aglycon N-glycan_core_beta-Man
- \forall is_aglycon_of (N-glycan_alpha-Man_8 \sqcup N-glycan_alpha-Man_11 \sqcup N-glycan_beta-glcNAc_9 \sqcup N-glycan_beta-glcNAc_10 \sqcup N-glycan_beta-glcNAc_12)
- is_linked_to_aglycon_via \exists "O6"
- anomeric_carbon \exists 1
- has_absolute_configuration \exists D
- has_aglycon = 1
- has_aglycon \leq 1
- has_anomeric_configuration \exists alpha [from alpha-D-mannopyranosyl_residue]
- has_configuration \exists manno [from mannosyl_residue]
- has_main_chain_carbons \exists 6 [from hexosyl_residue]
- has_ring_form \exists pyranoid [from pyranosyl_residue]
- has_sugar_structural_variant \exists aldo [from aldo_sugar_residue]

All instances are aglycon of the union of

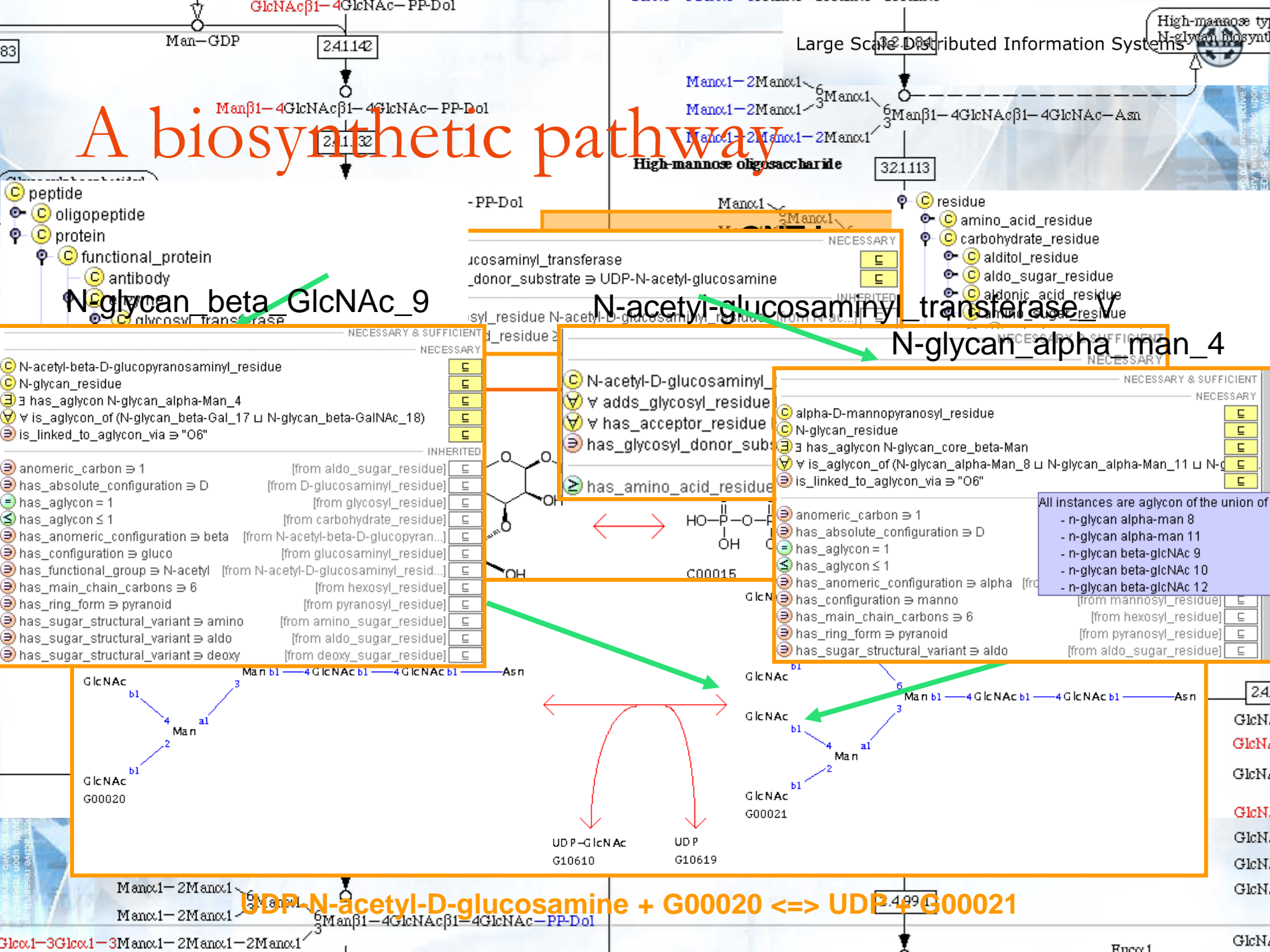
- n-glycan alpha-man 8
- n-glycan alpha-man 11
- n-glycan beta-glcNAc 9
- n-glycan beta-glcNAc 10
- n-glycan beta-glcNAc 12

Properties at Class

- ☒ is_linked_to_aglycon_via
- ☐ has_absolute_configuration
- ☐ has_aglycon
- ☐ has_configuration
- ☐ has_ring_form
- ☐ has_sugar_structural_variant
- ☒ anomeric_carbon
- ☐ has_carbohydrate_residue
- ☒ has_main_chain_carbons

Disjoints

A biosynthetic pathway

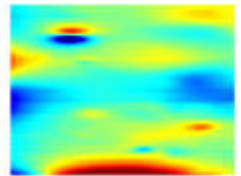
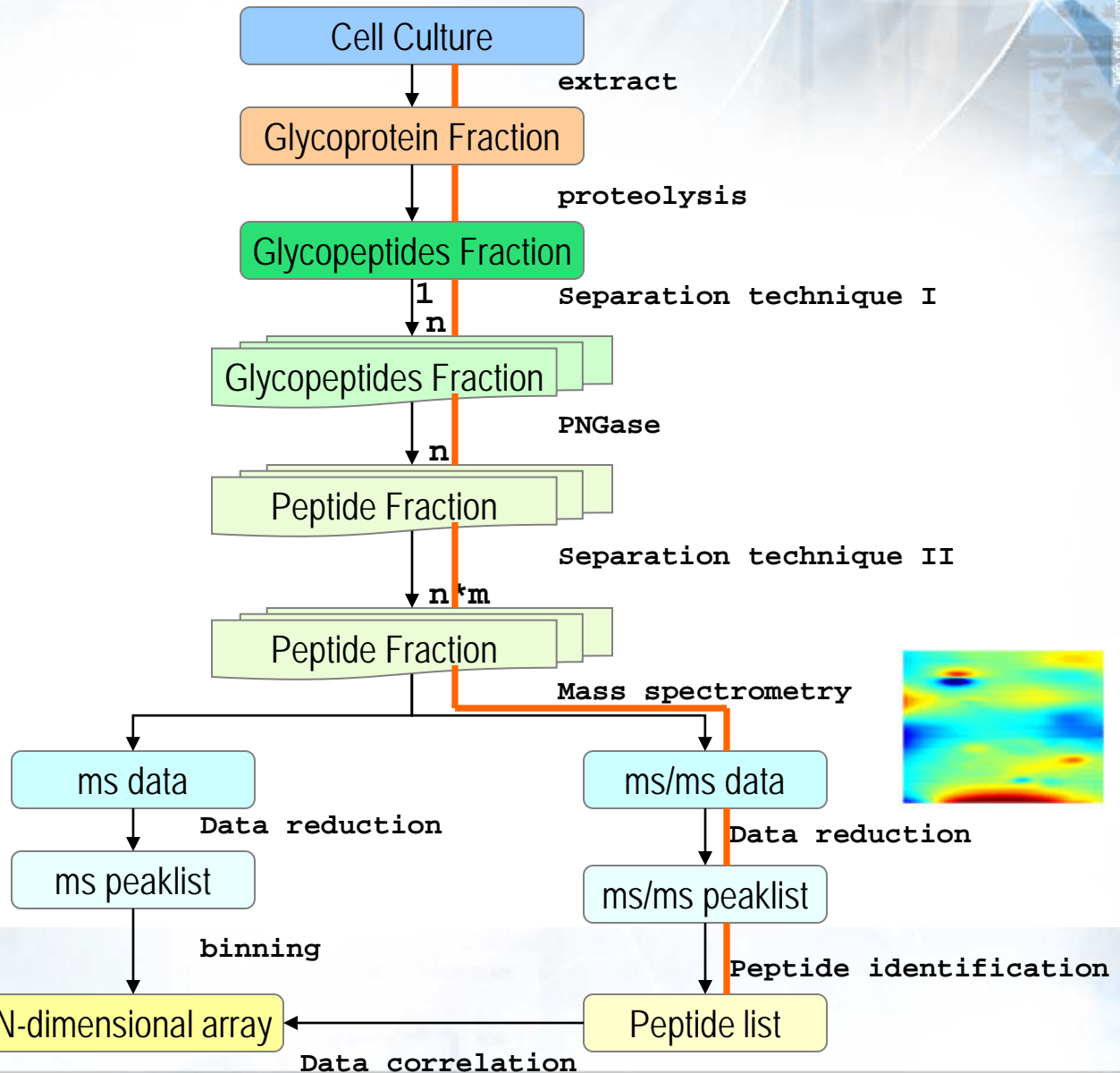
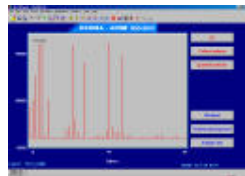
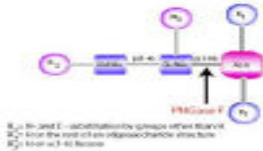




Proteomics Process Ontology - ProPreO

- A process ontology to capture proteomics experimental lifecycle: Separation, Mass spectrometry, Analysis
- 340 classes with 200+ properties
- proteomics experimental data include:
 - a) Data Provenance
 - b) Comparability of data, metadata (parameters settings for a HPLC run) and results
 - c) Finding implicit relationship between data sets using relations in the ontology – leading to indirect but critical interactions perhaps leading to knowledge discovery

N-Glycosylation Process (NGP)



Glycopeptide identification and quantification

Signal integration



Semantic Annotation of Scientific Data

```
830.9570 194.9604 2
580.2985 0.3592
688.3214 0.2526
779.4759 38.4939
784.3607 21.7736
1543.7476 1.3822
1544.7595 2.9977
1562.8113 37.4790
1660.7776 476.5043
```

ms/ms peaklist data

```
<ms/ms_peak_list>
<parameter
  instrument=micromass_QTOF_2_quadropole_time_of_flight_m
  ass_spectrometer
  mode = "ms/ms"/>
<parent_ion_mass>830.9570</parent_ion_mass>
<total_abundance>194.9604</total_abundance>
<z>2</z>
<mass_spec_peak m/z = 580.2985 abundance = 0.3592/>
<mass_spec_peak m/z = 688.3214 abundance = 0.2526/>
<mass_spec_peak m/z = 779.4759 abundance = 38.4939/>
<mass_spec_peak m/z = 784.3607 abundance = 21.7736/>
<mass_spec_peak m/z = 1543.7476 abundance = 1.3822/>
<mass_spec_peak m/z = 1544.7595 abundance = 2.9977/>
<mass_spec_peak m/z = 1562.8113 abundance = 37.4790/>
<mass_spec_peak m/z = 1660.7776 abundance = 476.5043/>
</ms/ms_peak_list>
```

Annotated ms/ms peaklist data

Two of the most active
very (which builds upon
TEOS's *Sustainable Web*

```
<ms/ms_peak_list>
<parameter
instrument="micromass_QTOF_2_quadropole_time_of_flight_mass_s
pectrometer"
mode = "ms/ms"/>
<parent_ion_mass>830.9570</parent_ion_mass>
<total_abundance>194.9604</total_abundance>
<z>2</z>
<mass_spec_peak m/z = 580.2985 abundance = 0.3592/>
<mass_spec_peak m/z = 688.3214 abundance = 0.2526/>
<mass_spec_peak m/z = 779.4759 abundance = 38.4939/>
<mass_spec_peak m/z = 784.3607 abundance = 21.7736/>
<mass_spec_peak m/z = 1543.7476 abundance = 1.3822/>
<mass_spec_peak m/z = 1544.7595 abundance = 2.9977/>
<mass_spec_peak m/z = 1562.8113 abundance = 37.4790/>
<mass_spec_peak m/z = 1660.7776 abundance = 476.5043/>
</ms/ms_peak_list>
```

Annotated ms/ms peaklist data

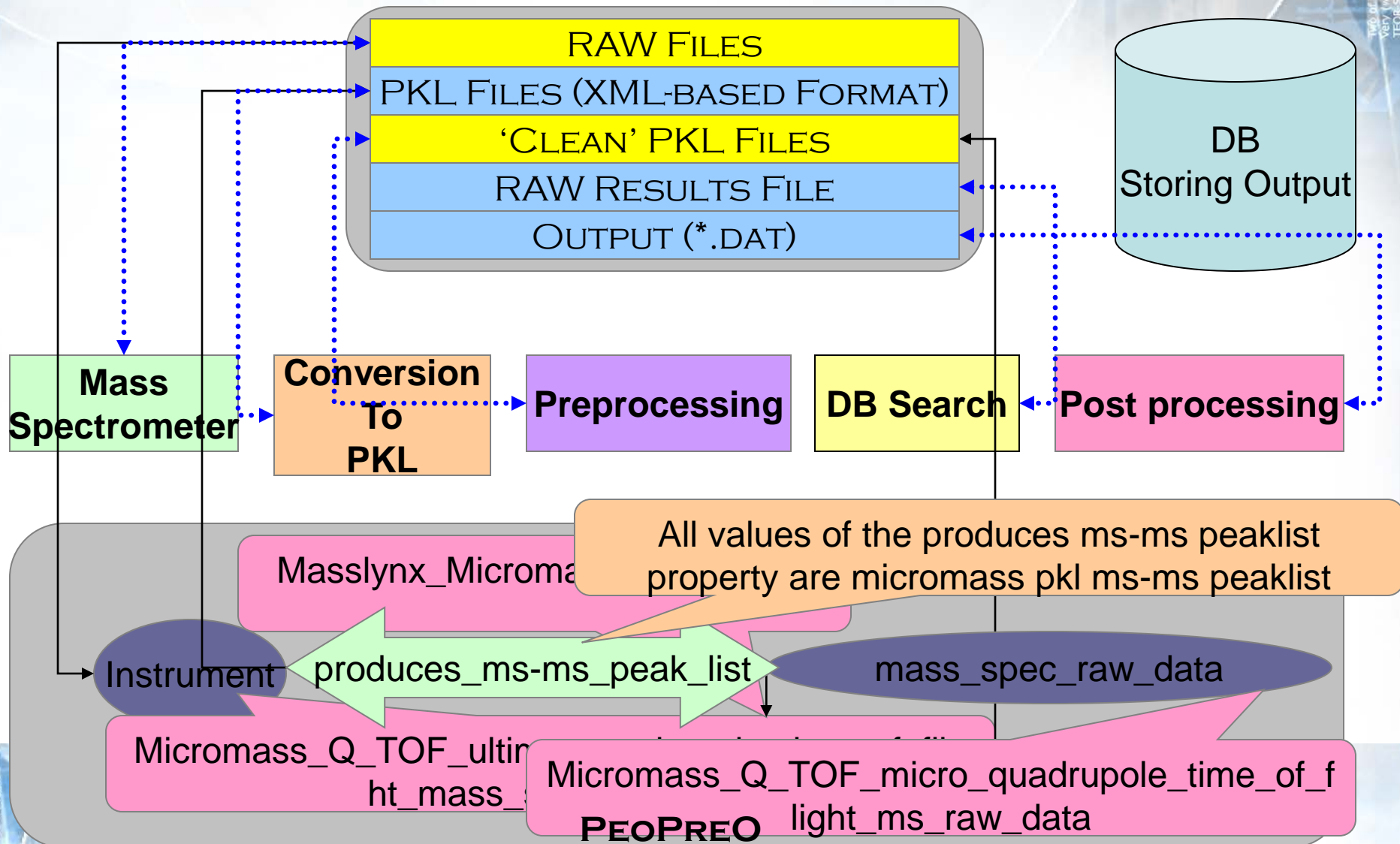


Beyond Provenance.... Semantic Annotations

- ❑ Data provenance: information regarding the '*place of origin*' of a data element
- ❑ Mapping a data element to concepts that collaboratively define it and enable its interpretation – Semantic Annotation
- ❑ Data provenance paves the path to repeatability of data generation, but it does not enable:
 - Its (machine) interpretability
 - Its computability (e.g., discovery)Semantic Annotations make these possible.



Ontology-mediated Proteomics Protocol





Service description using WSDL-S

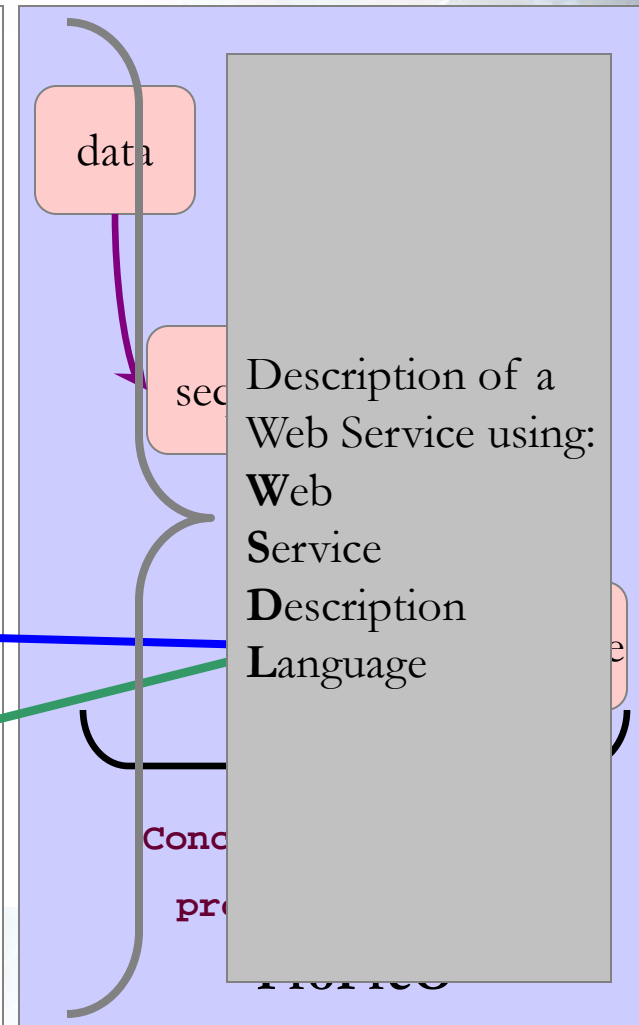
- ❖ Formalize description and classification of Web Services using ProPreO concepts

```

<?xml version="1.0" encoding="UTF-8"?>
<wsdl:definitions targetNamespace="urn:ngp"
.....
  xmlns:
wssem="http://www.ibm.com/xmlns/WebServices/WSSemantics"
  xmlns:
ProPreO="http://lsdis.cs.uga.edu/ontologies/ProPreO.owl" >

<wsdl:types>
  <schema targetNamespace="urn:ngp"
    xmlns="http://www.w3.org/2001/XMLSchema">
.....
  </complexType>
  </schema>
</wsdl:types>
  <wsdl:message name="replaceCharacterRequest"
wssem:modelReference="ProPreO#peptide_sequence">
    <wsdl:part name="in0" type="soapenc:string"/>
    <wsdl:part name="in1" type="soapenc:string"/>
    <wsdl:part name="in2" type="soapenc:string"/>
  </wsdl:message>

```





Biological UDDI (BUDDI) WS Registry for Proteomics and Glycomics

- ❖ There are no current registries that use semantic classification of Web Services in glycoproteomics
- ❖ BUDDI classification based on proteomics and glycomics classification – part of integrated glycoproteomics Web Portal called [Stargate](#)
- ❖ NGP to be published in BUDDI
- ❖ Can enable other systems such as ^{my}Grid to use NGP Web Services to build a glycomics workbench



Summary, Observations, Conclusions

- Ontology Schema: relatively simple in business/industry, highly complex in science
- Ontology Population: could have millions of assertions, or unique features when modeling complex life science domains
- Ontology population could be largely automated if access to high quality/curated data/knowledge is available; ontology population involves disambiguation and results in richer representation than extracted sources
- Ontology freshness (and validation—not just schema correctness but knowledge—how it reflects the changing world)



Summary, Observations, Conclusions

- Ontology types: (upper), (broad base/ language support), (common sense), domain, task, process, ...
- Much of power of semantics is based on knowledge that populates ontology (schema by themselves are of little value)
- Some applications: semantic search, semantic integration, semantic analytics, decision support and validation (e.g., error prevention in healthcare), knowledge discovery, process/pathway discovery, ...



Advertisement

- IJSWIS (International Journal for Semantic Web & Information Systems) welcomes not only research but also vision, application (with evaluation/validation) and vision papers

More details on Industry Applications of SW: <http://www.semagix.com>; on Scientific Applications of SW: <http://lsdis.cs.uga.edu>